EFFECTS OF Ni_3Ti (DO_{24}) PRECIPITATES AND COMPOSITION ON Ni-BASED SUPERALLOYS USING MOLECULAR DYNAMICS METHOD

GOH KIAN HENG

UNIVERSITI TEKNOLOGI MALAYSIA

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GOH KIAN HENG

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ABSTRACT

The main aim of this study is to simulate and investigate the gamma and gamma prime phases structure stability and behaviour of misfit dislocation-precipitate with additional of Ni_3Ti (DO_{24}) in Ni-based superalloys using MD at 10 K, 293 K and 1000 K. The Ni_3Ti are homogeneously distributed through γ phase and the percentages are varied from 0.22%, 0.5%, 0.89% and 2.11%. MD is capable to produce three dimensions modelling based on time evolution of a set of interacting atoms and integrating their equation of motion. The Embedded Atom Method (EAM) is used to calculate phase stability, point defect properties, surface energies and relaxation for Ni-Ti-Al system. The empirical embedding energy function, electron density function and interatomic pair potential function used by this method are obtained. The conclusion of this simulation shows that distribution of Ni_3Ti is vital in determining the Ni-Ni_3Al phase stability. The data of temperature, total energy, stress in x-axis, stress in y-axis, stress in z-axis and volume are plotted and snapshot of each percentage of Ni_3Ti added is taken at different step. At higher temperature (1000 K), it is more favourable and stable condition for higher Ti concentration (9L 2.11%) because of lower energy level and more stable temperature condition.

ABSTRAK

Tujuan utama kajian ini adalah untuk menjalankan proses simulasi bagi menyiasat kestabilan fasa dan ketidakpadanan struktur gamma dan gamma prime serta kehelan-mendakan dengan penambahan Ni_3Ti (DO_{24}) dalam superalloys berasaskan Nickel menggunakan Molecular Dynamic (MD) pada 10 K, 293 K and 1000 K. Ni_3Ti diedarkan secara serata melalui fasa γ dengan peratusan penambahan Ni_3Ti diubah dari 0.22%, 0.5%, 0.89% and 2.11%. MD berupaya untuk menghasilkan pemodelan 3 dimensi yang berdasarkan evolusi masa satu set atom yang berinteraksi sesama sendiri dan mengintegrasikan persamaan pergerakan yang terlibat. Embedded Atom Method (EAM) digunakan untuk mengira kestabilan fasa, ciri-ciri kecacatan titik, tenaga permukaan dan kelonggaran untuk sistem Ni-Ti-Al. Fungsi tenaga pembenaman empirikal, fungsi ketumpatan elektron dan fungsi potensi pasangan atom yang digunakan melalui kaedah ini, dapat diperolehi. Kesimpulannya, hasil daripada proses simulasi ini menunjukkan bahawa pembahagian Ni_3Ti adalah sangat penting dalam menentukan kestabilan fasa Ni-Ni_3Al. Data suhu, jumlah tenaga, tekanan di x-paksi, tekanan di paksi-y, tekanan di paksi-z dan isipadu diplotkan dan gambar setiap peratusan Ni_3Ti diambil pada langkah yang berbeza. Pada suhu yang lebih tinggi (1000 K), keadaan ada lebih sesuai dan stabil bagi peratusan Ti yang lebih tinggi (9L 2.11%) kerana jumlah tenaga ada lebih rendah dan keadaan suhu yang lebih stabil.